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# USER'S GUIDE FOR TRAN72 COMPUTER CODE MODIFIED FOR USE WITH RAMP AND VOFMOC FLOWFIELD CODES. Users Guide,

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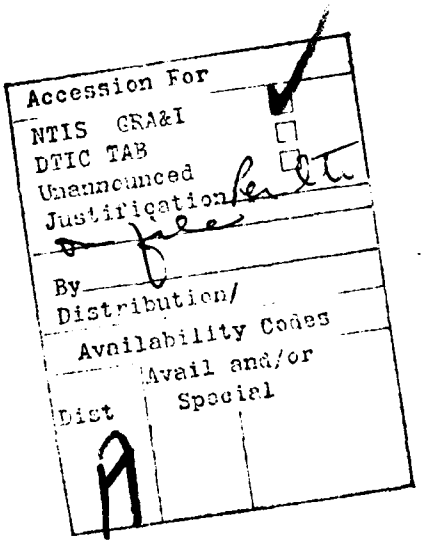
# FOREWORD

This document presents the results of work performed by personnel of the Fluid Mechanics Section of Lockheed's Huntsville Research & Engineering Center. This document was prepared for the Engineering Analysis Division of the NASA-Johnson Space Center, Houston, Texas under Contract NAS9-13429, Barney B. Roberts, technical monitor.



# INTRODUCTION AND SUMMARY

This document presents a description of the modifications made to the TRAN72 computer program to meet the general requirements of Lockheed's two-phase flow analysis computer programs (specifically the reacting multi-phase computer program), and provides instructions for operating the modified TRAN72 program.

The modified TRAN72 program is available for external distribution.

# Section 1
# CHEMICAL EQUILIBRIUM CALCULATION MODIFICATIONS

The TRAN72 computer program (developed by NASA-Lewis Research Center (Ref. 1)) was synthesized by combining a program for the transport properties calculation with the CEC 71 program (Ref. 2) for the thermodynamic properties calculation. The TRAN72 program was subsequently modified to meet the requirements of Lockheed's reacting multi-phase computer program, RAMP (Ref. 3). The requirements satisfied were: (1) calculation of the theoretical rocket performance (for both equilibrium and frozen compositions) during a "gaseous-only" expansion, after a two-phase combustion chamber calculation; (2) inclusion of a sudden pressure freeze during a two-phase equilibrium expansion calculation; and (3) automated communication of these properties to the RAMP program.

Modifications were made to the TRAN72 chemical equilibrium calculational scheme in order to generate thermochemical data consistent with the assumptions utilized in the RAMP program formulation. The assumptions being addressed in the RAMP program are:

- The total mass of the mixture is constant.
- The total energy of the mixture is constant.
- The gas obeys the perfect gas law and is either chemically frozen, in chemical nonequilibrium or in chemical equilibrium.
- There is no mass exchange between the phases.
- The particles are inert.

In the modified TRAN72 calculational scheme, the chamber calculations are performed initially with the condensed species considered. The total mass and total enthalpy of the mixture are then adjusted by removing the mass and enthalpy associated with the condensed species predicted to exist in the chamber

after combustion. The total mass adjustment is made by removing the appropriate amount of mass of each of the elements which comprise the condensed species that exist in the chamber. The total enthalpy is adjusted by removing the enthalpy associated with the condensed species that exist in the chamber. The adjusted elemental mass balance relationships and the adjusted total enthalpy are then referenced to the adjusted total mass of the mixture. All condensed species are then removed from the list of possible products being considered by the program. The chamber calculations and subsequent equilibrium chemistry expansion are then made with a gaseous-only composition. Upon completion of the thermodynamic calculations, the transport properties are calculated in the manner described in Ref. 1. The resultant equilibrium chemistry expansion and corresponding transport properties data are for the case in which there is no heat transfer between the condensed and gaseous species during the equilibrium chemistry expansion process. To account for the effects of the heat transfer that does take place between the condensed and gaseous species during the flowfield calculations, additional thermochemical data is required. To generate the required data, the total enthalpy of the gaseous-only mixture is perturbed (mass is held constant) and the thermochemical data calculational scheme is repeated. The total enthalpy is repeatedly perturbed; the result being an array of equilibrium expansion processes and corresponding transport properties, each with a different degree of heat transfer between the two phases.

Past experience in thermodynamical modeling of rocket exhaust flows has indicated that many chemical systems experience a transition from equilibrium to frozen chemistry during the expansion process. The standard TRAN72 program has an existing option to treat this problem. Under the pressure freeze option the chamber and initial expansion calculations are made assuming equilibrium chemistry. At a predetermined pressure ratio (chamber to local static) the chemistry of the system is frozen and the remainder of the expansion is completed with frozen chemistry. With this option, the transport properties are calculated in the manner outlined in Ref. 1.

The thermochemical and transport data are communicated to the RAMP computer program automatically through the use of a magnetic tape (or rapid access storage, i.e., disc, FASTRAN, etc.). Creation of the data tape (or file) is accomplished by means of an additional subroutine (MOCDAT) added to the TRAN72 program. Logic is provided in this routine for creation of a new data tape (or file) and adding data to an existing Master data list. Each data case must be identified with a unique case name which is subsequently used by the RAMP program to determine if thermodynamic data are available. An additional namelist has been added to the run stream to control use of the options available in the MOCDAT subroutine.

The modified TRAN72 program is used to generate thermodynamic and transport properties of the gaseous phase of the products of combustion being considered in a two-phase flow analysis. Control of the program function for this application is handled through three input groups: the reactant data cards, the $INPT2 namelist, and the $RKTINP namelist. A detailed description of the standard TRAN72 program input is given in Ref. 1. The thermodynamic data required for this application are calculated using the RKT option under the $INPT2 namelist. Selection of this option permits calculation of theoretical rocket performance for both equilibrium and frozen compositions during expansions. The variables MOC2P, PARTHT, QDOTP and NQI have been added to the $INPT2 namelist. The MOC2P variable controls the selection of the two-phase flow analysis option (MOC2P=T). The variables PARTHT, QDOTP and NQI control the selection (PARTHT=T) and use of the variable total enthalpy option when the effects of heat transfer between the condensed and gaseous species are to be determined in a two-phase flow analysis. When PARTHT=T, QDOTP is set equal to the amount by which the total enthalpy of the gaseous-only mixture is to be perturbed. NQI is set equal to the number of QDOTP values input. The specific values of the ratio of chamber to local static pressures ($P_c/P$) at which thermodynamic and transport data are generated are input to the program in the $RKTINP namelist. The pressure freeze option is activated by setting the variable NFZ under the $RKTINP namelist equal to the number of the pressure ratio at which transition from equilibrium to frozen chemistry is to occur. (The chamber is considered to

be number one, the throat number two, etc.). Freeze pressures may be the chamber value or any supersonic pressure. No provision is made for freeze pressures between chamber and throat. The parameters which are generally utilized by the RAMP program are local Mach number, static pressure and temperature, isentropic coefficient (gamma), molecular weight, entropy, Prandtl number, viscosity, specific heat at constant pressure and the total enthalpy (gas only). These parameters, with the exception of the total enthalpy, are calculated for each value of ($P_c$/P) ratio by the program. A detailed description of the logic involved in the standard TRAN72 program computation is presented in flow chart form in Ref. 1. This information can be consulted for an in-depth understanding of the calculational scheme.

To automatically create a tape for communication with the RAMP program requires that one of the two tape-write options be selected (MOCT=T, or MOCTF=T) under the $INPT2 namelist. The MOCT variable is utilized when the thermochem data are to be run completely under the equilibrium assumption. The MOCTF variable is utilized when the thermochem data are to be run completely or partially frozen. If one of these options is selected an additional namelist, $TAPGEN, must be input to control the tape-write function and the input of the case name card. The $TAPGEN data are input after the $INPT2 data but prior to the case name card and $RKTINP namelist inputs. Table 1 summarizes the program variables added to the modified TRAN72 program.

Four example cases showing the required input format for creation of thermodynamic data for typical rocket performance problems are presented in Table 2. Case 1 is the required input to perform a calculation of theoretical rocket performance for both the equilibrium and frozen composition assumptions during an isentropic expansion. (No tape is generated.) Case 2 is the same as Case 1 except that a tape for communication with other programs is generated for the frozen composition assumption during expansion (MOCTF=T). Case 3 is the required input format for creation of thermodynamic data for use with the RAMP program (MOC2P=T); a tape is generated

Table 1

ADDITIONAL INPUT VARIABLES FOR MODIFIED* TRAN72 PROGRAM

| $INPT2 NAMELIST | | | | | |
|---|---|---|---|---|---|
| Variable | Dimension | Type | Common Label | Value Before Read | Comment |
| MOCT | 1 | L | HREC | F | Selects tape-write option if true for equil. run. |
| MOC2P | 1 | L | HREC | F | Selects two-phase flow analysis option if true. |
| MOCTF | 1 | L | HREC | F | Selects tape-write option if true for frozen and pressure freeze options. |
| PARTHT | 1 | L | TWOPAS | F | Selects variable total enthalpy option if true for two-phase analysis run. |
| QDOTP** | 26 | R | TWOPAS | 0.0 | Set equal to the amount by which the total enthalpy of the gaseous-only mixture is to be perturbed. |
| NQI | 1 | I | TWOPAS | 0 | Set equal to the number of QDOTP values input. |
| $TAPGEN NAMELIST | | | | | |
| IREAD | 1 | I | — | 1 | If equal 0, new data added to master data tape list; if equal 1 data written on new data tape. |
| IO | 1 | I | — | 8 | Tape unit of old master tape list. |
| IN*** | 1 | I | — | 10 | Tape unit of new data tape. |
| Case Name Card Format: 6A4 | | | | | |

*Routines modified from the original TRAN72 program are: LINK, MAIN1 REACT, SEARCH, EQLBRM, ROCKET, RKTOUT, OUT1, TRANSP, OUT.

**The values of QDOTP must always be input in ascending order (from the most negative to the most positive).

***When running multiple cases, the data of the last case must always be placed on tape unit 10 if it is to be communicated automatically to the RAMP or VOFMOC programs.

Table 2

EXAMPLE CASES SHOWING THE REQUIRED INPUT FORMAT FOR CREATION OF THERMODYNAMIC DATA FOR TYPICAL ROCKET PERFORMANCE PROBLEMS

Case 1: Required input to perform a calculation of theroretical rocket performance for both the equilibrium and frozen composition assumptions during expansion. (No tape is generated.)

```
REACTANTS
H  2.00                                          1.00      0.0        6298.15   R
O  2.00                                          1.00      0.0        6298.15   O
                    (Insert Blank Card)
NAMELISTS
 $INPT2
      RKT=T,PSIA=T,CASE=00001,P=200.00,OF=T,MIX=0.0
 $END
 $RKTINP
  PCP=10.,30.,50.,100.,500.,1000.,5000.,50000.,100000.,500000.
 $END
```

Case 2: Same as Case 1 except that a tape for communication with other programs is generated for the frozen composition assumption during expansion (MOCTF=T).

```
REACTANTS
H  2.00                                          1.00      0.0        6298.15   R
O  2.00                                          1.00      0.0        6298.15   O
                    (Insert Blank Card)
NAMELISTS
 $INPT2
      RKT=T,PSIA=T,CASE=00001,P=200.00,OF=T,MIX=0.0,MOCTF=T
 $END
 $TAPGEN
      IREAD=1,IO=8,IN=10
 $END
 CASE 2
 $RKTINP
  PCP=10.,30.,50.,100.,500.,1000.,5000.,50000.,100000.,500000.
 $END
```

Table 2 (Continued)

Case 3: Required input for creation of thermodynamic data for use with the RAMP program (MOC2P=T); a tape is generated for the equilibrium composition assumption during expansion (MOCT=T). (The effects of heat transfer between the condensed and gaseous species are not determined.)

```
REACTANTS
AL 1.0                                                    16.      0.0       S298.15  F
C 6.884  H 10.089 O .278   N .264                         12.04    -12000.   S298.15  F
FE2.0    O 3.0                                             .4      -197300.  S298.15  F
C 6.15   H  6.97  O 1.17   N .03                           1.96     -28300.   S298.15  F
N 1.0    H  4.0   O 4.0    CL 1.0                         69.60    -70690.   S298.15  F
                    (Insert Blank Card)
OMIT          AL(S)          AL(L)          ALCL3(S)          ALCL3(L)
OMIT          ALN(S)         ALN            AL2CL6            AL2O2
OMIT          CCL3           CCL4           CH                CH2
OMIT          CH3            CH4            COCL2             C2CL2
OMIT          C2H6           C3O2           C4                C5
OMIT          FE(S)          FE(L)          FECL2(S)          FECL2(L)
OMIT          H2O(S)         H2O(L)
NAMELISTS
 $INPT2
      RKT=T,PSIA=T,KASE=00001,P=554.00,MOC2P=T,MOCT=T
 $END
 $TAPGEN
      IREAD=1,IO=8,IN=10
 $END
 CASE 3
 $RKTINP
  PCP=10.,30.,50.,100.,500.,1000.,5000.,50000.,100000.,500000.
 $END
```

Case 4: Same as Case 3 except that the effects of heat transfer between the condensed and gaseous species are determined (PARTHT=T).

```
REACTANTS
AL 1.0                                                    16.      0.0       S298.15  F
C 6.884  H 10.089 O .278   N .264                         12.04    -12000.   S298.15  F
FE2.0    O 3.0                                             .4      -197300.  S298.15  F
C 6.15   H  6.97  O 1.17   N .03                           1.96     -28300.   S298.15  F
N 1.0    H  4.0   O 4.0    CL 1.0                         69.60    -70690.   S298.15  F
                    (Insert Blank Card)
OMIT          AL(S)          AL(L)          ALCL3(S)          ALCL3(L)
OMIT          ALN(S)         ALN            AL2CL6            AL2O2
OMIT          CCL3           CCL4           CH                CH2
OMIT          CH3            CH4            COCL2             C2CL2
OMIT          C2H6           C3O2           C4                C5
OMIT          FE(S)          FE(L)          FECL2(S)          FECL2(L)
OMIT          H2O(S)         H2O(L)
NAMELISTS
 $INPT2
      RKT=T,PSIA=T,KASE=00001,P=554.00,MOC2P=T,MOCT=T,PARTHT=T,
      GOOTP=-600.0,-300.0,0.0,0.0,100.0,NGI=4
 $END
 $TAPGEN
      IREAD=1,IO=8,IN=10
 $END
 GOOTP TEST CASE
 $RKTINP
  PCP=10.,30.,50.,100.,500.,1000.,5000.,50000.,100000.,500000.
 $END
```

for the equilibrium composition assumption during the isentropic expansion (MOCT=T). (The effects of heat transfer between the condensed and gaseous species are not determined.) *Finally, Case 4 is the same as Case 3 except* that the effects of heat transfer between the condensed and gaseous species are determined (PARTHT=T).

## 2.2 USE OF THE MODIFIED TRAN72 PROGRAM WITH THE STANDARD VOFMOC PROGRAM

The TRAN72 program has been modified to meet the requirements of the RAMP computer program. The data tape (or file) created for communication with the ramp program contains additional data not required by the VOFMOC program (Ref. 4). For that reason, the tape read statement and format statement in subroutines GASTAP and GASRD, respectively, must be modified to read the additional data as "dummy" variables. The following statements must be changed in the above subroutines before the data tape generated by the TRAN72 program can be read correctly by the VOFMOC program.

- Subroutine GASRD

Old Statement: `1 FORMAT(4A6,5X,A3,6X,I2,3X,I2)`

New Statement: `1 FORMAT(6A4,5X,A3,6X,I2,3X,I2)`

- Subroutine GASTAP

Old Statement: `10 READ(10)(BETA(I),I=1,4),IOF,IS`

New Statement: `10 READ(10)(BETA(I),I=1,4),DU,DU,IOF,IS`

There are no other limitations placed on the use of the modified TRAN72 program. Further assistance on running the program may be obtained from the authors.

## CONCLUSIONS

The TRAN72 computer code (Ref. 1) has been modified by Lockheed-Huntsville personnel to provide thermochemical data that are compatible with the RAMP computer code assumptions. The basic capability of the code has been left undisturbed. Thermochemical composition analyses check cases have been run on the ABMDA 7600 and on the Univac 1108 Exec 8 at Huntsville, Alabama.

The TRAN72 program is a large-scale scientific endeavor with great capability and flexibility. Programs of this size however, are rarely finished but usually undergo periodic revision to increase capability, incorporate system changes and corrections of defects which might occur in untested situations. With this in mind, it is suggested that any receiving organization address questions concerning the basic TRAN72 program to the authors of Ref. 1. Questions concerning the TRAN72 modifications should be directed to the Lockheed-Huntsville authors at the following address:

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Huntsville Research & Engineering Center
P. O. Box 1103
Huntsville, Alabama 35807

## REFERENCES

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